Graduate Student Research Seminar

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Impact of Nanoparticle Surface Configurations on the Mechanical Properties of Polymer Nanocomposites

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3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Nanoparticle-reinforced polymer nanocomposites have gained attention for their tunable mechanical properties, but the impact of nanoparticle surface configurations on mechanical properties of polymer nanocomposites remains underexplored due to computational and experimental challenges. Using coarse-grained molecular dynamics simulations, this study investigates the effects of smooth, corrugated, and porous nanoparticle surfaces on the mechanical performance of polymethyl methacrylate (PMMA) nanocomposites. Specifically, we conduct tensile, shear, and small amplitude oscillatory shear tests to characterize the nanocomposites' stiffness and damping-related properties depending on surface configurations. The results show that the nanoparticle-PMMA nanocomposites outperforms pure PMMA in both Young's and shear moduli, with porous nanoparticles providing the greatest enhancement. Increased interfacial interactions between the nanoparticle and PMMA matrix are strongly correlated with improved mechanical performance. A quasilinear relationship is observed between the nanocomposite shear modulus and Debye-Waller factor-based molecular stiffness, with porous nanoparticles exhibiting the highest stiffness. Furthermore, local molecular stiffness analysis reveals significant dynamic heterogeneity, particularly in porous nanoparticle systems with strong interfacial interactions. Small amplitude oscillatory tests reveal simultaneous improvements in G', G'', and $\tan(\delta)$ with increasing nanoparticle surface roughness and interfacial interactions. This finding is notable as it defies the typical tradeoff between stiffness and damping capability. We attribute the enhanced damping capability to pronounced dynamic heterogeneity associated with rougher nanoparticle surfaces and interfacial interactions. This study demonstrates that tailoring nanoparticle surface configurations can optimize the mechanical properties of nanocomposites and overcome traditional stiffness-damping tradeoff.

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